

Non–Markovian diffusion over potential barrier in the presence of periodic time modulation

V. M. Kolomietz and S. V. Radionov

Institute for Nuclear Research, 03680 Kiev, Ukraine

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Abstract

The diffusive non–Markovian motion over a single–well potential barrier in the presence of a weak sinusoidal time–modulation is studied. We found non–monotonic dependence of the mean escape time from the barrier on a frequency of the periodic modulation that is character to the stochastic resonance phenomenon. The resonant acceleration of diffusion over the barrier occurs at the frequency inversely proportional to the mean first–passage time for the motion in the absence of the time–modulation.

I. INTRODUCTION

The response of complex nonlinear systems on periodic time input may have the features that are absent for linear systems. The very famous example of such features is the stochastic resonance phenomenon [1], when the response of the nonlinear system on the harmonic perturbation is resonantly activated under some optimal level of a noise. The resonant activation of the system occurs when the frequency of the modulation is near the Kramers' escape rate of the transitions from one potential well to another. The stochastic resonance phenomenon has been found and studied in many physical systems like a ring laser [2], magnetic systems [3], optical bistable systems [4] and others. The prototype of the stochastic resonance studies is a model of overdamped motion between potential wells of the bistable system. The frequency of the transitions between wells is given by the famous Kramers' rate and the stochastic resonance is achieved when a frequency of an external periodic modulation is of the order of the Kramers' rate.

In the present paper, we would like to study a diffusion over a single-well potential barrier in the presence of periodic time modulation. The diffusion over the barrier is generated by a colored noise whose statistical properties are related to the retarded friction term. In addition to the works [5]–[7], we are going to study how the correlation time of the colored noise influence the first passage time distribution and escape rate over the barrier.

The paper is organized as follows. In Sect. II, we set in basic Langevin equation of motion for diffusive motion over a potential barrier in the presence of sinusoidal time modulation. In Sect. III A, it is considered the unperturbed path of the model system. The time modulated diffusion is discussed in Sect. III B. Finally, the main conclusions of the paper are given in Sect. IV.

II. DIFFUSIVE MOTION OVER A POTENTIAL BARRIER

We start from a quite general Langevin formulation of the problem of diffusive overcoming of a potential barrier in the presence of a harmonic perturbation $V_{\text{ext}}(t) = \alpha \cdot \sin(\omega t)$:

$$M\ddot{q}(t) = -\frac{\partial E_{\text{pot}}}{\partial q} - \int_0^t \kappa(t-t')\dot{q}(t')dt' + \xi(t) + \alpha \cdot \sin(\omega t), \quad (1)$$

where q is the dimensionless coordinate, M is the mass, $\kappa(t - t')$ is the memory kernel and $\xi(t)$ is the random force. The potential energy E_{pot} is schematically shown in Fig. 1 and presents a single-well barrier formed by a smoothing joining at $q = q^*$ of the potential minimum oscillator with the inverted oscillator,

$$\begin{aligned} E_{\text{pot}} &= \frac{1}{2}M\omega_A^2(q - q_A)^2, \quad q \leq q^*, \\ &= E_{\text{pot,B}} - \frac{1}{2}M\omega_B^2(q - q_B)^2, \quad q > q^*. \end{aligned} \quad (2)$$

A noise term $\xi(t)$ in Eq. (1) is assumed to be Gaussian distributed with zero mean and correlation function related to a memory kernel $\kappa(t - t')$ of a retarded friction force:

$$\langle \xi(t) \xi(t') \rangle = T \kappa(t - t'). \quad (3)$$

Below we shall assume that the memory kernel is given by

$$\kappa(t - t') = \kappa_0 \exp\left(-\frac{|t - t'|}{\tau}\right), \quad (4)$$

where τ is a correlation time.

III. NUMERICAL CALCULATIONS

In the numerical calculations, we have measured all quantities of the dimension of energy in units of the temperature of the system $E_0 = T$, quantities of the dimension of time in units of $t_0 = \sqrt{M/T}$ and quantities of the dimension of frequency in units of $\omega_0 = \sqrt{T/M}$. For the system's parameters q_A , q^* , q_B , ω_A , ω_B , $E_{\text{pot,B}}$ and κ_0 , we adopted the values:

$$\begin{aligned} q_A &= 1, \quad q^* = 1.2, \quad q_B = 1.6, \\ \omega_A &= 6.75, \quad \omega_B = 9.59, \quad E_{\text{pot,B}} = 5.15, \quad \kappa_0 = 1920. \end{aligned} \quad (5)$$

which are widely used under model diffusion-like studies of fission of highly excited atomic nuclei, see Ref. [8].

A. Unperturbed diffusion over the barrier

At the beginning, we investigated the non-Markovian diffusive dynamics for the infinitely slow ($\omega = 0$) modulation and calculated a first-passage time distribution. For that, the Langevin equation (1) was solved numerically by generating a bunch of the trajectories, all starting at the potential well (point A in Fig. 1) and having the initial velocities distributed according to the Maxwell-Boltzman distribution. First, we would like to study the diffusive dynamics (1)–(4) in terms of first passage time distribution.

In Fig. 2, the mean first-passage time is presented as a function of the correlation time τ .

An increase of the mean first-passage time t_{mfpt} with the relaxation time τ means that memory effects in the Langevin dynamics (1) hinders the diffusion over the barrier. A non-monotonic growth of the mean first-passage time is caused by transition (occurred at the $\tau \approx 0.007$) from nearly Markovian regime of the diffusion (1) to the regime where the memory effects are quite important. As far as the memory effects become stronger and stronger ($\tau \rightarrow \infty$), the value of t_{mfpt} reaches a finite limit. Here, the hindrance of the escape over the barrier is caused by the renormalization of the ordinary conservative force in Eq. (1) that obtains an additional contribution from the time-retarded force

$$-\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt' \rightarrow -\kappa_0 [q(t) - q_A], \quad \tau \rightarrow \infty. \quad (6)$$

In the opposite limit of quite small values of the correlation time τ , the hindrance is exclusively due to an usual friction:

$$-\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt' \rightarrow -\kappa_0 \tau \dot{q}(t), \quad \tau \rightarrow 0. \quad (7)$$

In intermediate case, the hindrance is defined both by the friction and the additional elastic force,

$$-\kappa_0 \int_0^t \exp\left(-\frac{|t-t'|}{\tau}\right) \dot{q}(t') dt' = -\gamma(t, \tau) \dot{q}(t) - C(t, \tau) q(t), \quad (8)$$

where the effective friction coefficient $\gamma(t, \tau)$ may be quite well approximated by

$$\gamma(t, \tau) \approx \frac{\kappa_0 \cdot \tau}{1 + (\kappa_0/M)\tau^2}, \quad t \gg \tau. \quad (9)$$

The stiffness parameter $C(t, \tau)$ in Eq. (8) grows from 0 to κ_0 with a growing of τ .

Secondly, we measure the diffusion dynamics (1)–(4) through an escape rate, $R(t)$, characteristics. The escape rate over the barrier is defined as follows

$$R(t) = -\frac{1}{P(t)} \frac{dP(t)}{dt}, \quad (10)$$

where $P(t)$ is the survival probability, i.e., probability of finding the system on the left from the top of the barrier up to time t :

$$P(t) = N(t)/N_0. \quad (11)$$

Here, $N(t)$ is a number of the trajectories being not reaching the top of the barrier up to time t and N_0 is a total number of the trajectories involved in the calculations. In Fig. 3, it is plotted the typical time behavior of the escape rate $R(t)$ for quite small $\tau = 0.005$ and fairly large $\tau = 0.026$ values of the correlation time.

It is seen from Fig. 3 that initially the escape is affected by transient effects, when the survival probability $P(t)$ deviates strongly from the exponential form. With time, the escape process becomes more and more stationary giving rise to the corresponding saturation of the rate $R(t)$ (10) establishing of a quasistationary probability flow over the barrier. Qualitatively, one can describe typical time evolution of the escape rate as

$$R(t) = R_0(1 - e^{-t/t_{\text{tran}}}). \quad (12)$$

In both cases a duration of the transient period, t_{tran} , is almost the same ($t_{\text{tran}} \approx 50$) for quite weak and fairly large memory effects in the diffusion process. However, a saturation value, R_0 , of the escape rate is significantly different. It is because of the memory effect for the large values of the correlation time τ .

In Fig. 4, we showed how the value R_0 (12) depends on the size of the memory effects in the diffusive dynamics (1). Dotted line in Fig. 4 represents the famous Kramers' result for the escape rate value in a quasistationary regime [9]

$$R_{Kr} = \frac{\omega_A}{2\pi} \left(\sqrt{1 + \left[\frac{\gamma(\tau)}{2M\omega_B} \right]^2} - \frac{\gamma(\tau)}{2M\omega_B} \right) \exp\left(-\frac{B}{T}\right), \quad (13)$$

where the τ -dependent friction coefficient $\gamma(\tau)$ is given by Eq. (9).

We see that the memory effects significantly suppress the value of the escape rate in the saturation regime of probability flow over the potential barrier. Initially (i. e., at relatively small values of the correlation time τ) the suppression is mainly caused by the growing role of the usual friction in the non-Markovian diffusion (1)–(4), see also Eqs. (8) and (9). As is followed from the Fig. 4, in this case the escape rate at saturation R_0 (12) may be quite well approximated by the Kramers' formula (13). On the other hand, at relatively large correlation times τ , the effect of the friction on the diffusion over the barrier is negligibly weak and the escape rate's suppression appears exclusively due to the additional conservative force, see Eq. (8). As a result, the stationary value of the escape rate deviates substantially from the Kramers' escape rate (13) at the fairly strong memory effects in the diffusive motion across the barrier.

B. Diffusion over the barrier in the presence of a periodic modulation

Now we will study the diffusion over the barrier (1)–(4) in the presence of the external harmonic force. We will assume that the amplitude α of the force $\alpha \cdot \sin(\omega t)$ in Eq. (1) is so small ($\alpha = 0.05$) that still the reaching the top of the barrier is caused exclusively by diffusive nature of the process.

In Fig. 5, we calculated the typical dependencies of the mean first-passage time t_{mfpt} on the frequency ω of the external harmonic force. The calculations were performed for the weak, $\tau = 0.005$, (lower curve in Fig. 5) and strong, $\tau = 0.026$, (upper curve in Fig. 5) memory effect on the non-Markovian diffusive motion over the barrier.

In both cases the mean first-passage time t_{mfpt} non-monotonically depends on the frequency of the perturbation that is character for the stochastic resonance phenomenon observed in a number of different physical systems. From Fig. 5 one can conclude that diffusion over the potential barrier in the presence of the harmonic time perturbation is maximally accelerated at some definite so to say resonant frequency ω_{res} of the perturbation,

$$\omega_{\text{res}} \approx \frac{1.5}{t_{\text{mfpt}}(\omega = 0)} \quad (14)$$

see also Figs. 2 and 4. In fact, the quantity $t_{\text{mfpt}}(\omega = 0)$ presents the characteristic time scale for the diffusion dynamics (1). In the case of adiabatically slow time variations of the harmonic force, $\omega t_{\text{mfpt}}(\omega = 0) \ll 1$ and $t < t_{\text{mfpt}}$, one can approximately use $\alpha \cdot \sin(\omega t) \approx \alpha \cdot \omega t$

and the diffusion over the barrier is slightly accelerated. As a result of that, the mean first-passage time $t_{\text{mfpt}}(\omega)$ is smaller than the corresponding unperturbed value $t_{\text{mfpt}}(\omega = 0)$. The same feature is also observed at the fairly large modulation's frequencies. Thus, in the case of $\omega t_{\text{mfpt}}(\omega = 0) \gg 1$, the harmonic perturbation $\alpha \cdot \sin(\omega t)$ may be treated as a random noise term with the zero mean value and variance α^2 . Such a new stochastic term will lead to additional acceleration of the diffusion over the barrier.

The existence of the resonant regime (14) in the periodically modulated diffusion process (1) is even more clear visible in the escape rate characteristics of the process. We have plotted in Fig. 6 the time evolution of the escape rate (10) found for the resonant frequency ω_{res} (14) (curve 1 in Fig. 6), the quite smaller frequency $\omega = \omega_{\text{res}}/10$ (curve 2 in the Fig. 6) and the quite larger frequency $\omega = 10 \omega_{\text{res}}$ (curve 3 in Fig. 6) of the modulation.

Again, at very slow ($\omega = \omega_{\text{res}}/10$) and fast ($\omega = 10\omega_{\text{res}}$) perturbations the escape rate $R(t)$ looks very similar to the corresponding unperturbed value $R(t, \omega = 0)$, compare Figs. 3 and 6. In other words, the initial transient period in the time evolution of the escape rate is followed by the stationary regime, when the escape subsequently saturates with time. Contrary to that, the escape rate shows complex time behavior as far as the periodic modulation occurs at the resonant frequency ($\omega = \omega_{\text{res}}$), see curve 1 in Fig. 6. This resonant regime of the modulated diffusion is essentially nonstationary when the system remains excited during quite long time. We checked such a feature for larger number of trajectories and longer time intervals used to calculate the escape rate characteristics (10).

IV. CONCLUSIONS

In the present study, we have investigated how model non-Markovian diffusion over the single-well parabolic barrier is affected by the external periodic time modulation. We have calculated both the mean first-passage time t_{mfpt} and the escape rate $R(t)$ over the barrier. These two quantities have been found to be sensitive to the relative size of memory effects in the diffusive dynamics (1)–(4), measured by the correlation time τ . Thus, we have demonstrated that the memory effects hinder the escape over the barrier, see Figs. 2 and 4. In contrast to the motion in the presence of usual friction force, the hindrance of the escape occurs due to the Markovian friction and additional conservative components (8) of the retarded time force in Eq. (1). Having calculated the mean first-passage time t_{mfpt} for

different values of the frequency ω of the modulation, we have found that the sinusoidal perturbation accelerates the diffusion over the barrier, see Fig. 5. The maximal (resonant) acceleration is achieved at the $\omega = \omega_{\text{res}}$, where ω_{res} is inversely proportional to the mean first-passage time in the absence of the modulation (14). We have seen that a value of the resonant activation over the barrier $t_{\text{mfpt}}(\omega = \omega_{\text{res}})/t_{\text{mfpt}}(\omega = 0)$ remains practically the same for the quite weak as well as for the fairly strong memory effects in the diffusive dynamics. It has been observed that the diffusive dynamics (1)–(4) in the resonant activation regime (14) has the peculiarity, reflecting in the complex time behavior of the escape rate $R(t)$, see Fig. 6. Importantly, that the absence of the escape rate’s saturation with time implies essentially transient character of the events of the first passing the top of the potential barrier.

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Figure captions.

Fig. 1. Landscape of potential energy $E_{\text{pot}}(q)$ of Eq. (2).

Fig. 2. The mean first-passage time t_{mfpt} of the non-Markovian diffusion process (1)–(4) vs the correlation time τ .

Fig. 3. The time dependence of the escape rate $R(t)$ (10) of the non-Markovian diffusion process (1)–(4) calculated for the cases of quite small $\tau = 0.005$ and fairly large $\tau = 0.026$ values of the correlation time.

Fig. 4. The saturation value R_0 of the escape rate (10)–(12) vs the strength τ of the memory effects in the non-Markovian diffusion process (1)–(4). The dotted line represents the Kramers' result (13) for the escape rate calculated with the τ -dependent friction coefficient of Eq. (9).

Fig. 5. The mean first-passage time t_{mfpt} of the non-Markovian diffusion process (1)–(4) is given as a function of the frequency ω of the harmonic time perturbation at two values of the correlation time $\tau = 0.005$ (lower curve) and $\tau = 0.026$ (upper curve).

Fig. 6. The time dependence of the escape rate R (10) for the periodically modulated diffusion over the barrier (1)–(4) are shown at the resonant frequency ω_{res} (14) (curve 1), fairly smaller frequency $\omega = \omega_{\text{res}}/10$ (curve 2) and quite bigger frequency $\omega = 10\omega_{\text{res}}$ (curve 3) of the periodic modulation. The dependencies were calculated for the memory time $\tau = 0.01$.











